

Theoretical and Computational Molecular Science

P. PONGPRAYOON and T. MORI, “Critical Role of Dimer Formation in Monosaccharide Binding to Human Serum Albumin,” *Phys. Chem. Chem. Phys.* **20**, 3249–3257 (2018).

M. KALATHINGAL, T. SUMIKAMA, T. MORI, S. OIKI and S. SAITO, “Structure and Dynamics of Solvent Molecules inside Polytheonamide B Channel in Different Environments: A Molecular Dynamics Study,” *Phys. Chem. Chem. Phys.* **20**, 3334–3348 (2018).

M. OKUDA, M. HIGASHI, K. OHTA, S. SAITO and K. TOMINAGA, “Theoretical Investigation on Vibrational Frequency Fluctuations of SCN-Derivatized Vibrational Probe Molecule in Water,” *Chem. Phys.* **512**, 82–87 (2018).

T. YANAI, M. SAITOW, X.-G. XIONG, Y. KURASHIGE, J. CHALUPSKÝ, S. GUO and S. SHARMA, “Multi-State Complete Active-Space Second-Order Perturbation Theory with Density Matrix Renormalization Group Reference Wave Functions,” *J. Chem. Theory Comput.* **13**, 4829–4840 (2017). DOI: 10.1021/acs.jctc.7b00735

J. WEN, T. UTO, J. CHALUPSKÝ, D. L. CASHER, G. RAABE, J. FLEISCHHAUER, T. YANAI, H. TSUJI, K. KOMATSU and J. MICHL, “Magnetic Circular Dichroism of an Unaromatic Planar [8]Annulene,” *J. Phys. Org. Chem.* **31(8)**, e3854 (16 pages) (2018). DOI: 10.1002/poc.3854

R. D. REYNOLDS, T. YANAI and T. SHIOZAKI, “Large-Scale Relativistic Complete Active Space Self-Consistent Field with Robust Convergence,” *J. Chem. Phys.* **149**, 014106 (8 pages) (2018).

Y. FUJIHASHI, M. HIGASHI and A. ISHIZAKI, “Intramolecular Vibrations Complement the Robustness of Primary Charge Separation in a Dimer Model of the Photosystem II Reaction Center,” *J. Phys. Chem. Lett.* **9**, 4921–4929 (2018).

A. KATO and A. ISHIZAKI, “Non-Markovian Quantum-Classical Ratchet for Ultrafast Long-Range Electron–Hole Separation in Condensed Phases,” *Phys. Rev. Lett.* **121**, 026001 (5 pages) (2018).

N. T. PHUC and A. ISHIZAKI, “Control of Excitation Energy Transfer in Condensed Phase Molecular Systems by Floquet Engineering,” *J. Phys. Chem. Lett.* **9**, 1243–1248 (2018).

K. BOBUATONG, H. SAKURAI and M. EHARA, “Intramolecular Hydroamination by a Primary Amine of an Unactivated Alkene on Gold Nanoclusters: A DFT Study,” *ChemCatChem* **9**, 4490–4500 (2017).

P. ZHAO, X. ZHAO and M. EHARA, “Theoretical Insight into Sc₂C₇₆: Carbide Clusterfullerene Sc₂C₂@C₇₄ versus Dimetallofullerene Sc₂@C₇₆,” *Inorg. Chem.* **56**, 10195–10203 (2017).

R. ZHAO, K. YUAN, S. ZHAO, M. EHARA, S. NAGASE, J. M. POBLET and X. ZHAO, “Deciphering the Role of Long-Range Interaction in Endohedral Metallofullerenes: A Revisit to Sc₂C₇₀,” *J. Phys. Chem. C* **121**, 20481–20488 (2017).

R. ZHAO, K. YUAN, S. ZHAO, X. ZHAO and M. EHARA, “Quantum Chemical Insight into La₂C₉₆: Metal Carbide Fullerene La₂C₂@C₉₄ versus Dimetallofullerene La₂@C₉₆,” *Inorg. Chem.* **56**, 11883–11890 (2017).

K. TAKAGI, K. ITO, Y. YAMADA, T. NAKASHIMA, R. FUKUDA, M. EHARA and H. MASU, “Synthesis and Optical Properties of Excited-State Intramolecular Proton Transfer Active π -Conjugated Benzimidazole Compounds: Influence of Structural Rigidification by Ring Fusion,” *J. Org. Chem.* **82**, 12173–12180 (2017).

T. IWASAKI, A. FUKUOKA, W. YOKOYAMA, X. MIN, I. HISAKI, T. YANG, M. EHARA, H. KUNIYASU and N. KAMBE, “Nickel-Catalyzed Coupling Reaction of Alkyl Halides with Aryl Grignard Reagents in the Presence of 1,3-Butadiene: Mechanistic Studies of Four-Component Coupling and Competing Cross-Coupling Reactions,” *Chem. Sci.* **9**, 2195–2211 (2018).

T. SHIRAOGAWA, M. EHARA, S. JURINOVICH, L. CUPELLINI and B. MENNUCCI, “Frenkel-Exciton Decomposition Analysis of Circular Dichroism and Circularly Polarized Luminescence for Multichromophoric Systems,” *J. Comput. Chem.* **39**, 931–935 (2018).

P. ZHAO, X. ZHAO and M. EHARA, “Theoretical Insights into Monometallofullerene Th@C₇₆: Strong Covalent Interaction between Thorium and Carbon Cage,” *Inorg. Chem.* **57**, 2961–2964 (2018).

T. SOMMERFELD, J. B. MELUGIN and M. EHARA, “Temporary Anion States of Ethene Interacting with Single Molecules of Methane, Ethane, and Water,” *J. Phys. Chem. A* **122**, 2580–2586 (2018).

K. TAKAGI, Y. YAMADA, R. FUKUDA, M. EHARA and D. TAKEUCHI, “ESIPT Emission Behavior of Methoxy-Substituted 2-Hydroxyphenylbenzimidazole Isomers,” *New J. Chem.* **42**, 5923–5928 (2018).

S. KINOSHITA, Y. MIYAZAKI, M. SHIMADA, Y. ONITSUKA, H. KOHGUCHI, Y. INOKUCHI, N. AKAI, T. SHIRAOGAWA, M. EHARA, K. YAMAZAKI, Y. HARABUCHI, S. MAEDA, T. TAKETSUGU and T. EBATA, “Different Photoisomerization Routes Found in the Structural Isomers of Hydroxy Methylcinnamate,” *Phys. Chem. Chem. Phys.* **20**, 17583–17598 (2018).

A. JUNKAEW, S. NAMUANGRUK, P. MAITARAD and M. EHARA, “Silicon-Coordinated Nitrogen-Doped Graphene as a Promising Metal-Free Catalyst for N₂O Reduction by CO: A Theoretical Study,” *RSC Adv.* **8**, 22322–22330 (2018).

T. IWASAKI, X. MIN, A. FUKUOKA, L. ZHU, R. QIU, T. YANG, M. EHARA, A. SUDALAI and N. KAMBE, “Ni-Catalyzed Dimerization and Hydroperfluoroarylation of 1,3-Dienes,” *J. Org. Chem.* **83**, 9267–9277 (2018).

R. FUKUDA, S. SAKAI, N. TAKAGI, M. MATSUI, M. EHARA, S. SAKAKI, S. HOSOKAWA and T. TANAKA, “Mechanisms of NO–CO Reaction over Highly Dispersed Cuprous Oxide on γ -Alumina Catalyst Using Metal-Support Interfacial Site in the Presence of Oxygen: Similarity to and Difference from Biological Systems,” *Catal. Sci. Technol.* **8**, 3833–3845 (2018).

Y. MORI, H. OKUMURA, T. WATANABE and T. HOHSAKA, “Antigen-Dependent Fluorescence Response of Anti-c-Myc Quenchbody Studied by Molecular Dynamics Simulations,” *Chem. Phys. Lett.* **698**, 223–226 (2018).

H. NISHIZAWA and H. OKUMURA, “Classical Molecular Dynamics Simulation to Understand Role of a Zinc Ion for Aggregation of Amyloid- β Peptides,” *J. Comput. Chem., Jpn.* **17**, 76–79 (2018).

LIST OF PUBLICATIONS

M. YAMAUCHI and H. OKUMURA, “Development of Isothermal-Isobaric Replica-Permutation Method for Molecular Dynamics and Monte Carlo Simulations and Its Application to Reveal Temperature and Pressure Dependence of Folded, Misfolded, and Unfolded States of Chignolin,” *J. Chem. Phys.* **147**, 184107 (15 pages) (2017).

T. FUJITA and Y. MOCHIZUKI, “Development of the Fragment Molecular Orbital Method for Calculating Nonlocal Excitations in Large Molecular Systems,” *J. Phys. Chem. A* **122**, 3886–3898 (2018).

M. ZHOU, C. ZENG, M. Y. SFEIR, M. COTLET, K. IIDA, K. NOBUSADA and R. JIN, “Evolution of Excited-State Dynamics in Periodic Au₂₈, Au₃₆, Au₄₄, and Au₅₂ Nanoclusters,” *J. Phys. Chem. Lett.* **8**, 4023–4030 (2017).

T. YATSUI, H. SAITO, K. NISHIOKA, B. LEUSCHEL, O. SOPPERA and K. NOBUSADA, “Effects of a Power and Photon Energy of Incident Light on Near-Field Etching Properties,” *Appl. Phys. A: Mater. Sci. Process.* **123**, 751 (6 pages) (2017).

T. YATSUI, M. YAMAGUCHI and K. NOBUSADA, “Nano-Scale Chemical Reactions Based on Non-Uniform Optical Near-Fields and Their Applications,” *Prog. Quantum Electron.* **55**, 166–194 (2017).

T. YATSUI, H. SAITO and K. NOBUSADA, “Angstrom-Scale Flatness Using Selective Nano-Scale Etching,” *Beilstein J. Nanotechnol.* **8**, 2181–2185 (2017).

K. KOIZUMI, M. HATAKEYAMA, M. BOERO, K. NOBUSADA, H. HORI, T. MISONOU and S. NAKAMURA, “How Seaweeds Release the Excess Energy from Sunlight to Surrounding Sea Water,” *Phys. Chem. Chem. Phys.* **19**, 15745–15753 (2017).

H. MATSUI, S. ITO and M. NAKANO, “Open-Shell Character Dependences of Second Hyperpolarizability in Two-Dimensional Tetraradicaloids,” *J. Phys. Chem. A* **122**, 3680–3687 (2018).

S. TAKAMUKU and M. NAKANO, “Diradical Character and Second Hyperpolarizability of Alkali Earth Metal Inverse Sandwich Complexes Involving Cyclopentadienyl and Cyclooctatetraene Ligands,” *Eur. J. Inorg. Chem.* **2018**, 2894–2899 (2018).

S. MUHAMMAD, M. NAKANO, A. AL-SEHEMI, A. CHAUDHARY, A. IRFAN, T. TONAMI, R. KISHI, Y. KITAGAWA and S. ITO, “Exploring the Novel Donor-Nanotube Archetype as Efficient Third-Order Nonlinear Optical Material: Asymmetric Open-Shell Carbon Nanotubes,” *Nanoscale* **10**, 16345–16944 (2018).

T. NAGAMI, J. FUJIYOSHI, T. TONAMI, K. WATANABE, K. OKADA, R. KISHI, M. NAKANO, B. CHAMPAGNE and V. LIÉGEOIS, “Evaluation of Aromaticity for Open-Shell Singlet Dicyclopenta-Fused Acenes and Polyacenes Based on Magnetically Induced Current,” *Chem. –Eur. J.* **24**, 13457–13466 (2018).

Photo-Molecular Science

M. NAGASAKA, H. YUZAWA and N. KOSUGI, “Intermolecular Interactions of Pyridine in Liquid Phase and Aqueous Solution Studied by Soft X-Ray Absorption Spectroscopy,” *Z. Phys. Chem.* **232**, 705–722 (2018).

M. NAGASAKA, H. YUZAWA, T. HORIGOME and N. KOSUGI, “Reliable Absorbance Measurement of Liquid Samples in Soft X-Ray Absorption Spectroscopy in Transmission Mode,” *J. Electron Spectrosc. Relat. Phenom.* **224**, 93–99 (2018).

M. NAGASAKA, H. YUZAWA and N. KOSUGI, “Interaction between Water and Alkali Metal Ions and Its Temperature Dependence Revealed by Oxygen K-Edge X-Ray Absorption Spectroscopy,” *J. Phys. Chem. B* **121**, 10957–10964 (2017).

H. YAMANE, A. CARLIER and N. KOSUGI, “Orbital-Specific Electronic Interaction in Crystalline Films of Iron Phthalocyanine Grown on Au(111) Probed by Angle-Resolved Photoemission Spectroscopy,” *Mater. Chem. Front.* **3**, 609–614 (2018).

H. YAMANE and N. KOSUGI, “High Hole-Mobility Molecular Layer Made from Strong Electron Acceptor Molecules with Metal Adatoms,” *J. Phys. Chem. Lett.* **8**, 5366–5371 (2017).

M.-H. LI, H.-H. YEH, Y.-H. CHIANG, U.-S. JENG, C.-J. SU, H.-W. SHIU, Y.-J. HSU, N. KOSUGI, T. OHIGASHI, Y.-A. CHEN, P.-S. SHEN, P. CHEN and T.-F. GUO, “Highly Efficient 2D/3D Hybrid Perovskite Solar Cells via Low-Pressure Vapor-Assisted Solution Process,” *Adv. Mater.* **30**, 1801401 (13 pages) (2018).

Y. F. WANG, Y. C. SHAO, S. H. HSIEH, Y. K. CHANG, P. H. YEH, H. C. HSUEH, J. W. CHIOU, H. T. WANG, S. C. RAY, H. M. TSAI, C. W. PAO, C. H. CHEN, H. J. LIN, J. F. LEE, C. T. WU, J. J. WU, Y. M. CHANG, K. ASOKAN, K. H. CHAE, T. OHIGASHI, Y. TAKAGI, T. YOKOYAMA, N. KOSUGI and W. F. PONG, “Origin of Magnetic Properties in Carbon Implanted ZnO Nanowires,” *Sci. Rep.* **8**, 7758 (13 pages) (2018).

A. KHODABANDEH, R. D. ARRUA, B. R. COAD, T. RODEMANN, T. OHIGASHI, N. KOSUGI, S. C. THICKETT and E. F. HILDER, “Morphology Control in Polymerised High Internal Phase Emulsion Templated via Macro-RAFT Agent Composition: Visualizing Surface Chemistry,” *Polym. Chem.* **9**, 213–220 (2018).

T. GEJO, M. OURA, T. TOKUSHIMA, Y. HORIKAWA, H. ARAI, S. SHIN, V. KIMBERG and N. KOSUGI, “Resonant Inelastic X-Ray Scattering and Photoemission Measurement of O₂: Direct Evidence for Dependence of Rydberg-Valence Mixing on Vibrational States in O 1s-Rydberg States,” *J. Chem. Phys.* **147**, 044310 (7 pages) (2017).

C. YOU, F. XIA, Y. ZHAO, Y. ZHANG, Y. SHENG, Y. WU, X.-C. HANG, F. CHEN, H. MA, K. SHEN, Z. SUN, T. UEBA, S. KERA, C. ZHANG, H. ZHANG, Z.-K. CHEN and W. HUANG, “Probing Triplet Excited States and Managing Blue Light Emission of Neutral Tetradentate Platinum (II) Complexes,” *J. Phys. Chem. Lett.* **9**, 2285–2292 (2018).

Y. KASHIMOTO, K. YONEZAWA, M. MEISSNER, M. GRUENEWALD, T. UEBA, S. KERA, R. FORKER, T. FRITZ and H. YOSHIDA, “The Evolution of Intermolecular Energy Bands of Occupied and Unoccupied Molecular States in Organic Thin Films,” *J. Phys. Chem. C* **122**, 12090–12097 (2018).

C. GAUL, M. SCHWARZE, S. SCHELLHAMMER, F. BUSSOLOTTI, S. KERA, Z. BAO, G. CUNIBERTI, K. LEO and F. ORTMANN, “Efficient Organic Semiconductor Doping: Guidance from n-Doped C₆₀,” *Nat. Mater.* **17**, 439–444 (2018).

- C. GUO, S. SARKAR, S. REFAELY-ABRAMSON, D. A. EGGER, T. BENDIKOV, K. YONEZAWA, Y. SUDA, T. YAMAGUCHI, I. PECHT, S. KERA, N. UENO, M. SHEVES, L. KRONIK and D. CAHEN, "Electronic Structure of Dipeptides in the Gas-Phase and as an Adsorbed Monolayer," *Phys. Chem. Chem. Phys.* **20**, 6860–6867 (2018).
- M. SCHWARZE, B. D. NAAAB, M. L. TIETZE, R. SCHOLZ, P. PAHNER, F. BUSSOLOTTI, S. KERA, D. KASEMANN, Z. BAO and K. LEO, "Analyzing the n-Doping Mechanism of an Air-Stable Small-Molecule Precursor," *ACS Appl. Mater. Interfaces* **10**, 1340–1346 (2017).
- T. KANEYASU, Y. HIKOSAKA, M. FUJIMOTO, H. IWAYAMA, M. HOSAKA, E. SHIGEMASA and M. KATOH, "Observation of an Optical Vortex Beam from a Helical Undulator in the XUV Region," *J. Synchrotron Radiat.* **24**, 934–938 (2017).
- Y. TAIRA and M. KATOH, "Generation of Optical Vortices by Nonlinear Inverse Thomson Scattering at Arbitrary Angle Interactions," *Astrophys. J.* **860**, 45 (11 pages) (2018).
- S. MATSUBA, K. KAWASE, A. MIYAMOTO, S. SASAKI, M. FUJIMOTO, T. KONOMI, N. YAMAMOTO, M. HOSAKA and M. KATOH, "Generation of Vector Beam with Tandem Helical Undulators," *Appl. Phys. Lett.* **113**, 021106 (4 pages) (2018).
- S. CHO, B. S. KIM, B. KIM, W. KYUNG, J. SEO, M. PARK, J. W. JEON, K. TANAKA, J. D. DENLINGER, C. KIM, D. ODKHUU, B. H. KIM and S. R. PARK, "Electronic-Dimensionality Reduction of Bulk MoS₂ by Hydrogen Treatment," *Phys. Chem. Chem. Phys.* **20**, 23007–23012 (2018).
- T. NAKAMURA, Y. OHTSUBO, Y. YAMASHITA, S. IDETA, K. TANAKA, K. YAJI, A. HARASAWA, S. SHIN, F. KOMORI, R. YUKAWA, K. HORIBA, H. KUMIGASHIRA and S. KIMURA, "Giant Rashba Splitting of Quasi-One-Dimensional Surface States on Bi/InAs(110)-(2 × 1)," *Phys. Rev. B* **98**, 075431 (7 pages) (2018).
- N. MURAI, K. SUZUKI, S. IDETA, M. NAKAJIMA, K. TANAKA, H. IKEDA and R. KAJIMOTO, "Effect of Electron Correlations on Spin Excitation Bandwidth in Ba_{0.75}K_{0.25}Fe₂As₂ as Seen via Time-of-Flight Inelastic Neutron Scattering," *Phys. Rev. B* **97**, 241112(R) (6 pages) (2018).
- Y. SUGIYAMA, C. BERNARD, Y. OKUYAMA, S. IDETA, K. TANAKA, T. GREBER and T. HIRAHARA, "Flattening and Manipulation of the Electronic Structure of h-BN/Rh(111) Nanomesh upon Sn Intercalation," *Surf. Sci.* **672-673**, 33–38 (2018).
- T. ITO, D. PINEK, T. FUJITA, M. NAKATAKE, S. IDETA, K. TANAKA and T. OUISSE, "Electronic Structure of Cr₂AlC as Observed by Angle-Resolved Photoemission Spectroscopy," *Phys. Rev. B* **96**, 195168 (9 pages) (2018).
- F. MATSUI, H. OTA, K. SUGITA, M. MUNTWILER, R. STANIA and T. GREBER, "Parallel and Antiparallel Angular Momentum Transfer of Circularly Polarized Light to Photoelectrons and Auger Electrons at the Ni L₃ Absorption Threshold," *Phys. Rev. B* **97**, 035424 (6 pages) (2018).
- F. MATSUI, H. NISHIKAWA, H. DAIMON, M. MUNTWILER, M. TAKIZAWA, H. NAMBA and T. GREBER, "The 4π k_z Periodicity in Photoemission from Graphite," *Phys. Rev. B* **97**, 045430 (6 pages) (2018).
- F. MATSUI, T. MATSUSHITA and H. DAIMON, "Holographic Reconstruction of Photoelectron Diffraction and Its Circular Dichroism for Local Structure Probing," *J. Phys. Soc. Jpn.* **87**, 061004 (11 pages) (2018).
- T. OHIGASHI, A. ITO, K. SHINOHARA, S. TONE, Y. INAGAKI, H. YUZAWA and N. KOSUGI, "3-Dimensional Chemical Structures of an Isolated Cell Nucleus by a Scanning Transmission X-Ray Microscope," *Microsc. Microanal.* **24**, 400–401 (2018).
- M. M. SHIROLKAR, Y. F. WANG, Y. C. SHAO, K. H. CHEN, H. T. WANG, X. S. QUI, J. S. YANG, J. J. WU, J. W. CHIOU, T. OHIGASHI, N. KOSUGI and W. F. PONG, "Probing the Electronic Structure of BiVO₄ Coated ZnO Nanodendrite Core-Shell Nanocomposite Using X-Ray Spectroscopic and Spatially Resolved Scanning Transmission X-Ray Microscopy Studies," *Microsc. Microanal.* **24**, 468–469 (2018).
- M. HUTTULA, M. PATANEN, R. PIISPANEN, T. OHIGASHI, N. KOSUGI, S. SWARAJ, R. BELKHOUE, A. PRANOVICH, T. JYSKE, P. KILPELAINEN, A. KARKONEN, R. KORPINEN, T. LAAKSO, S. VALKONEN and P. SARANPAA, "STXM Chemical Mapping of Norway Spruce Knotwood Lignans," *Microsc. Microanal.* **24**, 482–483 (2018).
- K. SHINOHARA, T. OHIGASHI, S. TONE, M. KADO and A. ITO, "Quantitative Analysis of Mammalian Chromosome by Scanning Transmission Soft X-Ray Microscopy," *Ultramicroscopy* **194**, 1–6 (2018).
- M.-H. LI, H.-H. YEH, Y.-H. CHIANG, U.-S. JENG, C.-J. SU, H.-W. SHIU, Y.-J. HSU, N. KOSUGI, T. OHIGASHI, Y.-A. CHEN, P.-S. SHEN, P. CHEN and T.-F. GUO, "Highly Efficient 2D/3D Hybrid Perovskite Solar Cells via Low-Pressure Vapor-Assisted Solution Process," *Adv. Mater.* **30**, 1801401 (13 pages) (2018).
- Y. F. WANG, Y. C. SHAO, S. H. HSIEH, Y. K. CHANG, P. H. YEH, H. C. HSUEH, J. W. CHIOU, H. T. WANG, S. C. RAY, H. M. TSAI, C. W. PAO, C. H. CHEN, H. J. LIN, J. F. LEE, C. T. WU, J. J. WU, Y. M. CHANG, K. ASOKAN, K. H. CHAE, T. OHIGASHI, Y. TAKAGI, T. YOKOYAMA, N. KOSUGI and W. F. PONG, "Origin of Magnetic Properties in Carbon Implanted ZnO Nanowires," *Sci. Rep.* **8**, 7758 (13 pages) (2018).
- A. KHODABANDEH, R. D. ARRUA, B. R. COAD, T. RODEMANN, T. OHIGASHI, N. KOSUGI, S. C. THICKETT and E. F. HILDER, "Morphology Control in Polymerised High Internal Phase Emulsion Templated via Macro-RAFT Agent Composition: Visualizing Surface Chemistry," *Polym. Chem.* **9**, 213–220 (2018).
- K. SHINOHARA, T. OHIGASHI, S. TONE, M. KADO and A. ITO, "Quantitative Study of Mammalian Cells by Scanning Transmission Soft X-Ray Microscopy," *J. Phys.: Conf. Ser.* **849**, 012003 (4 pages) (2017).
- K. TAKEMOTO, M. YOSHIMURA, T. OHIGASHI, Y. INAGAKI, H. NAMBA and H. KIHARA, "Application of Soft X-Ray Microscopy to Environmental Microbiology of Hydrophobic," *J. Phys.: Conf. Ser.* **849**, 012010 (4 pages) (2017).
- T. OHIGASHI, Y. INAGAKI, A. ITO, K. SHINOHARA and N. KOSUGI, "Investigation of Measurement Condition for 3-Dimensional Spectroscopy by Scanning Transmission X-Ray Microscopy," *J. Phys.: Conf. Ser.* **849**, 012044 (4 pages) (2017).

LIST OF PUBLICATIONS

H. SUGA, S. KIKUCHI, Y. TAKEICHI, C. MIYAMOTO, M. MIYAHARA, S. MITSUNOBU, T. OHGIASHI, K. MASE, K. ONO and Y. TAKAHASHI, "Spatially Resolved Distribution of Fe Species around Microbes at the Submicron Scale in Natural Bacteriogenic Iron Oxides," *Microbes Environ.* **32**, 283–287 (2017).

H. IWAYAMA, C. LÉONARD, F. LE QUÉRÉ, S. CARNIATO, R. GUILLEMIN, M. SIMON, M. N. PIANCASTELLI and E. SHIGEMASA, "Different Time Scales in the Dissociation Dynamics of Core-Excited CF₄ by Two Internal Clocks," *Phys. Rev. Lett.* **119**, 203203 (5 pages) (2017).

T. KANEYASU, Y. HIKOSAKA, M. FUJIMOTO, H. IWAYAMA, M. HOSAKA, E. SHIGEMASA and M. KATOH, "Observation of an Optical Vortex Beam From a Helical Undulator in the XUV Region," *J. Synchrotron Radiat.* **24**, 934–938 (2017).

T. KANEYASU, Y. HIKOSAKA, M. FUJIMOTO, H. IWAYAMA, M. HOSAKA, E. SHIGEMASA and M. KATOH, "Observation of an Optical Vortex Beam from a Helical Undulator in the XUV Region," *J. Synchrotron Radiat.* **24**, 934–938 (2017).

Materials Molecular Science

K. TAMASAKU, E. SHIGEMASA, Y. INUBUSHI, I. INOUE, T. OSAKA, T. KATAYAMA, M. YABASHI, A. KOIDE, T. YOKOYAMA and T. ISHIKAWA, "Nonlinear Spectroscopy with X-Ray Two-Photon Absorption in Metallic Copper," *Phys. Rev. Lett.* **121**, 083901 (5 pages) (2018).

Y. WAKISAKA, D. KIDO, H. UEHARA, Q. YUAN, S. TAKAKUSAGI, Y. UEMURA, T. YOKOYAMA, T. WADA, M. UO, T. SAKATA, O. SEKIZAWA, T. URUGA, Y. IWASAWA and K. ASAKURA, "A Demonstration of Pt L₃-Edge EXAFS Free from Au L₃ Edge Using Log-Spiral Bent Crystal Laue Analyzers," *Catalysts* **8**, 204 (6 pages) (2018).

T. YOKOYAMA, A. KOIDE and Y. UEMURA, "Local Thermal Expansions and Lattice Strains in Elinvar and Stainless Steel Alloys," *Phys. Rev. Mater.* **2**, 023601 (7 pages) (2018).

L. YU, Y. TAKAGI, T. NAKAMURA, O. SEKIZAWA, T. SAKATA, T. URUGA, M. TADA, Y. IWASAWA, G. SAMJESKÉ and T. YOKOYAMA, "Non-Contact Electric Potential Measurements of Electrode Components in Operating Polymer Electrolyte Fuel Cell by Near Ambient Pressure XPS," *Phys. Chem. Chem. Phys.* **19**, 30798–30803 (2017).

A. KOIDE and T. YOKOYAMA, "Effects of the Spin–Orbit Interaction in Chromium on the Oxygen K-Edge X-Ray Magnetic Circular Dichroism Spectra in CrO₂," *Phys. Rev. B* **96**, 144419 (9 pages) (2017).

T. NAKAMURA, T. IKOMA and K. YAMADA, "Recent Developments in Electron Spin Science and Technology in Japan," *Appl. Magn. Reson.* **49**, 755–756 (2018).

T. ENOMOTO, M. KONDO, M. ASADA, T. NAKAMURA and S. MASAOKA, "Near-IR Light-Induced Electron Transfer via Dynamic Quenching," *J. Phys. Chem. C* **122**, 11282–11287 (2018).

M. ASADA and T. NAKAMURA, "Magnetic Resonance Investigation for Possible Antiferromagnetic Subphase in (TMTTF)₂Br," *Phys. Rev. B* **96**, 125120 (6 pages) (2017).

N. SHINTAKU, S. IZAWA, K. TAKAGI, H. NAITO and M. HIRAMOTO, "Hole- and Electron-Only Transport in Ratio-Controlled Organic Co-Deposited Films Observed by Impedance Spectroscopy," *Org. Electron.* **50**, 515–520 (2017).

N. SHINTAKU, M. HIRAMOTO and S. IZAWA, "Effect of Trap-Assisted Recombination on Open-Circuit Voltage Loss in Phthalocyanine/Fullerene Solar Cells," *Org. Electron.* **55**, 69–74 (2018).

N. SHINTAKU, M. HIRAMOTO and S. IZAWA, "Controlling Open-Circuit Voltage in Organic Solar Cells by Impurity Doping," *J. Phys. Chem. C* **122**, 5248–5253 (2018).

S. IZAWA, N. SHINTAKU and M. HIRAMOTO, "Effect of Band Bending and Energy Level Alignment at the Donor/Acceptor Interface on Open-Circuit Voltage in Organic Solar Cells," *J. Phys. Chem. Lett.* **9**, 2914–2918 (2018).

M. HIRAMOTO, M. KIKUCHI and S. IZAWA, "Parts-per-Million-Level Doping Effects in Organic Semiconductor Films and Organic Single Crystals," *Adv. Mater.* 1801236 (15 pages) (2018). [Invited Progress Report]

A. NAITO, K. OKUSHITA, K. NISHIMURA, G. S. BOUTIS, A. AOKI and T. ASAKURA, "Quantitative Analysis of Solid-State Homonuclear Correlation Spectra of Antiparallel β -Sheet Alanine Tetramers," *J. Phys. Chem. B* **122**, 2715–2724 (2018).

K. ONO, S. KARASUDA and M. TOMURA, "Synthesis and Crystal Structure of 4⁵,8⁵-Di-*tert*-butyl-1,3,5,7(2,5)-tetraoxadiazola-2,6(2,6)-dipyridina-4,8(1,3)-dibenzenacyclooctaphane," *Heterocycles* **94**, 2209–2214 (2017).

E. TISSEROND, J. N. FUCHS, M. O. GOERBIG, P. AUBAN-SENZIER, C. MÉZIÈRE, P. BATAIL, Y. KAWASUGI, M. SUDA, H. M. YAMAMOTO, R. KATO, N. TAJIMA and M. MONTEVERDE, "Aperiodic Quantum Oscillations of Particle-Hole Asymmetric Dirac Cones," *EPL* **119**, 67001 (5 pages) (2017).

Life and Coordination-Complex Molecular Science

A. PAVLOU, A. LOULLIS, H. YOSHIMURA, S. AONO and E. PINAKOULAKI, “Probing the Role of the Heme Distal and Proximal Environment in Ligand Dynamics in the Signal Transducer Protein HemAT by Time-Resolved Step-Scan FTIR and Resonance Raman Spectroscopy,” *Biochemistry* **56**, 5309–5317 (2017).

A. PAVLOU, H. YOSHIMURA, S. AONO and E. PINAKOULAKI, “Protein Dynamics of the Sensor Protein HemAT as Probed by Time-Resolved Step-Scan FTIR Spectroscopy,” *Biophys. J.* **114**, 584–591 (2018).

T. KATO, K. KIKUTA, A. KANEMATSU, S. KONDO, H. YAGI, K. KATO and E. Y. PARK, “Alteration of a Recombinant Protein N-Glycan Structure in Silkworms by Partial Suppression of N-Acetylglucosaminidase Gene Expression,” *Biotechnol. Lett.* **39**, 1299–1308 (2017).

H. YAGI, H. TATENO, K. HAYASHI, T. HAYASHI, K. TAKAHASHI, J. HIRABAYASHI, K. KATO and M. TSUBOI, “Lectin Microarray Analysis of Isolated Polysaccharides from *Sasa veitchii*,” *Biosci., Biotechnol., Biochem.* **81**, 1687–1689 (2017).

R. YOGO, S. YANAKA, H. YAGI, A. MARTEL, L. PORCAR, Y. UEKI, R. INOUE, N. SATO, M. SUGIYAMA and K. KATO, “Characterization of Conformational Deformation-Coupled Interaction between Immunoglobulin G1 Fc Glycoprotein and a Low-Affinity Fcγ Receptor by Deuteration-Assisted Small-Angle Neutron Scattering,” *Biochem. Biophys. Rep.* **12**, 1–4 (2017).

T. SATOH, C. SONG, T. ZHU, T. TOSHIMORI, K. MURATA, Y. HAYASHI, H. KAMIKUBO, T. UCHIHASHI and K. KATO, “Visualisation of a Flexible Modular Structure of the ER Folding-Sensor Enzyme UGGT,” *Sci. Rep.* **7**, 12142 (10 pages) (2017).

S. KITAZAWA, M. YAGI-UTSUMI, K. KATO and R. KITAHARA, “Interactions Controlling the Slow Dynamic Conformational Motions of Ubiquitin,” *Molecules* **22**, 1414 (12 pages) (2017).

S. YANAKA, T. YAMAZAKI, R. YOGO, M. NODA, S. UCHIYAMA, H. YAGI and K. KATO, “NMR Detection of Semi-Specific Antibody Interactions in Serum Environments,” *Molecules* **22**, 1619 (8 pages) (2017).

Y. SAKAE, T. SATOH, H. YAGI, S. YANAKA, T. YAMAGUCHI, Y. ISODA, S. IIDA, Y. OKAMOTO and K. KATO, “Conformational Effects of N-Glycan Core Fucosylation of Immunoglobulin G Fc Region on Its Interaction with Fcγ Receptor IIIa,” *Sci. Rep.* **7**, 13780 (10 pages) (2017).

T. TAKENAKA, T. NAKAMURA, S. YANAKA, M. YAGI-UTSUMI, M. S. CHANDAK, K. TAKAHASHI, S. PAUL, K. MAKABE, M. ARAI, K. KATO and K. KUWAJIMA, “Formation of the Chaperonin Complex Studied by 2D NMR Spectroscopy,” *PLoS One* **12**, e0187022 (2017).

T. KOZAI, T. SEKIGUCHI, T. SATOH, H. YAGI, K. KATO and T. UCHIHASHI, “Two-Step Process for Disassembly Mechanism of Proteasome α7 Homo-Tetradecamer by α6 Revealed by High-Speed Atomic Force Microscopy,” *Sci. Rep.* **7**, 15373 (9 pages) (2017).

H. YAGI, G. YAN, T. SUZUKI, S. TSUGE, T. YAMAGUCHI and K. KATO, “Lewis X-Carrying Neoglycolipids Evoke Selective Apoptosis in Neural Stem Cells,” *Neurochem. Res.* **43**, 212–218 (2018).

M. YAGI-UTSUMI, A. SIKDAR, T. KOZAI, R. INOUE, M. SUGIYAMA, T. UCHIHASHI, H. YAGI, T. SATOH and K. KATO, “Conversion of Functionally Undefined Homopentameric Protein PbaA into a Proteasome Activator by Mutational Modification of Its C-Terminal Segment Conformation,” *Protein Eng., Des. Sel.* **31**, 29–36 (2018).

J. KICUNTOD, K. SANGPHEAK, M. MUELLER, P. WOLSCHANN, H. VIERNSTEIN, S. YANAKA, K. KATO, W. CHAVASIRI, P. PONGSAWASDI, N. KUNGWAN and T. RUNGROTMONGKOL, “Theoretical and Experimental Studies on Inclusion Complexes of Pinostrobin and β-Cyclodextrins,” *Sci. Pharm.* **86**, 5 (15 pages) (2018).

H. YAGI, D. TAKAKURA, L. T. ROUMENINA, W. H. FRIDMAN, C. SAUTÈS-FRIDMAN, N. KAWASAKI and K. KATO, “Site-Specific N-Glycosylation Analysis of Soluble Fcγ Receptor IIIb in Human Serum,” *Sci. Rep.* **8**, 2719 (7 pages) (2018).

K. KATO, T. FURUHASHI, K. KATO, A. ODA and E. KURIMOTO, “The Assembly Mechanism of Coiled-Coil Domains of the Yeast Cargo Receptors Emp46p/47p and the Mutational Alteration of pH-Dependency of Complex Formation,” *J. Biochem.* **163**, 441–446 (2018).

R. YOGO, S. YANAKA and K. KATO, “Backbone ¹H, ¹³C, and ¹⁵N Assignments of the Extracellular Region of Human Fcγ Receptor IIIb,” *Biomol. NMR Assignments* **12**, 201–204 (2018).

K. MUKAIGASA, T. TSUJITA, V. T. NGUYEN, L. LI, H. YAGI, Y. FUSE, Y. NAKAJIMA-TAKAGI, K. KATO, M. YAMAMOTO and M. KOBAYASHI, “Nrf2 Activation Attenuates Genetic Endoplasmic Reticulum Stress Induced by a Mutation in the Phosphomannomutase 2 Gene in Zebrafish,” *Proc. Natl. Acad. Sci. U.S.A.* **115**, 2758–2763 (2018).

N. SRIWILAJAROEN, S. NAKAKITA, S. KONDO, H. YAGI, K. KATO, T. MURATA, H. HIRAMATSU, T. KAWAHARA, Y. WATANABE, Y. KANAI, T. ONO, J. HIRABAYASHI, K. MATSUMOTO and Y. SUZUKI, “N-Glycan Structures of Human Alveoli Provide Insight into Influenza A Virus Infection and Pathogenesis,” *FEBS J.* **285**, 1611–1634 (2018).

S. YANAKA, H. YAGI, R. YOGO, M. YAGI-UTSUMI and K. KATO, “Stable Isotope Labeling Approaches for NMR Characterization of Glycoproteins Using Eukaryotic Expression Systems,” *J. Biomol. NMR* **71**, 193–202 (2018).

K. MORITA, Y. Y. YAMAMOTO, A. HORI, T. OBATA, Y. UNO, K. SHINOHARA, K. NOGUCHI, K. NOI, T. OGURA, K. ISHII, K. KATO, M. KIKUMOTO, R. ARRANZ, J. M. VALPUESTA and M. YOYODA, “Expression, Functional Characterization, and Preliminary Crystallization of the Cochaperone Prefoldin from the Thermophilic Fungus *Chaetomium thermophilum*,” *Int. J. Mol. Sci.* **19**, 2452 (13 pages) (2018).

A. NAKAMURA, T. TASAKI, Y. OKUNI, C. SONG, K. MURATA, T. KOZAI, M. HARA, H. SUGIMOTO, K. SUZUKI, T. WATANABE, T. UCHIHASHI, H. NOJI and R. IINO, “Rate Constants, Processivity, and Productive Binding Ratio of Chitinase A Revealed by Single-Molecule Analysis,” *Phys. Chem. Chem. Phys.* **20**, 3010–3018 (2018).

F. KAWAI, A. NAKAMURA, A. VISOOTSAT and R. IINO, “Plasmid-Based One-Pot Saturation Mutagenesis and Robot-Based Automated Screening for Protein Engineering,” *ACS Omega* **3**, 7715–7726 (2018).

T. UCHIHASHI, Y. H. WATANABE, Y. NAKAZAKI, Y. YAMASAKI, T. WATANABE, T. MARUO, S. UCHIYAMA, S. SONG, K. MURATA, R. IINO and T. ANDO, “Dynamic Structural States of ClpB Involved in Its Disaggregation Function,” *Nat. Commun.* **9**, 2147 (12 pages) (2018).

LIST OF PUBLICATIONS

- K. KATAYAMA, Y. FURUTANI, M. IWAKI, T. FUKUDA, H. IMAI and H. KANDORI**, “In situ” Observation of Role of Chloride Ion Binding to Monkey Green Sensitive Visual Pigment by ATR-FTIR Spectroscopy,” *Phys. Chem. Chem. Phys.* **20**, 3381–3387 (2018).
- A. SUEA-NGAM, M. SRISA-ART and Y. FURUTANI**, “PDMS-Based Microfluidic Device for Infrared-Transmission Spectro-Electrochemistry,” *Bull. Chem. Soc. Jpn.* **91**, 728–734 (2018).
- H. TSUKAMOTO, M. HIGASHI, H. MOTOKI, H. WATANABE, C. GANSER, K. NAKAJO, Y. KUBO, T. UCHIHASHI and Y. FURUTANI**, “Structural Properties Determining Low K^+ Affinity of the Selectivity Filter in the TWIK1 K^+ Channel,” *J. Biol. Chem.* **293**, 6969–6984 (2018).
- T. S. SYMEONIDIS, A. ATHANASOULIS, R. ISHII, Y. UOZUMI, Y. M. A. YAMADA and I. N. LYKAKIS**, “Photocatalytic Aerobic Oxidation of Alkenes into Epoxides or Chlorohydrins Promoted by a Polymer-Supported Decatungstate Catalyst,” *ChemPhotoChem* **1**, 478–484 (2017).
- Y. HIRAI and Y. UOZUMI**, “Preparation of Aryl(dicyclohexyl)phosphines by C–P Bond-Forming Cross-Coupling in Water Catalyzed by an Amphiphilic-Resin-Supported Palladium Complex,” *Synlett* **28**, 2966–2970 (2017).
- S. PAN, Y. SHUO, T. OSAKO and Y. UOZUMI**, “Batch and Continuous-Flow Huisgen 1,3-Dipolar Cycloadditions with An Amphiphilic Resin-Supported Triazine-Based Polyethyleneamine Dendrimer Copper Catalyst,” *ACS Sustainable Chem. Eng.* **5**, 10722–10734 (2017).
- T. OSAKO, K. TORII, S. HIRATA and Y. UOZUMI**, “Chemoselective Continuous-Flow Hydrogenation of Aldehydes Catalyzed by Platinum Nanoparticles Dispersed in an Amphiphilic Resin,” *ACS Catal.* **7**, 7371–7377 (2017).
- D. ROY and Y. UOZUMI**, “Recent Advances in Palladium-Catalyzed Cross-Coupling Reactions at ppm to ppb Molar Catalyst Loadings,” *Adv. Synth. Catal.* **360**, 602–625 (2018).
- A. OHTAKA, A. SAKON, A. YASUI, T. KAWAGUCHI, G. HAMASAKA, Y. UOZUMI, T. SHINAGAWA, O. SHIMOMURA and R. NOMURA**, “Catalytic Specificity of Linear Polystyrene-Stabilized Pd Nanoparticles during Ullmann Coupling Reaction in Water and the Associated Mechanism,” *J. Organomet. Chem.* **854**, 87–93 (2018).
- R. HUDSON, H. R. ZHANG, A. LOTEPLIO, G. BENEDETTO, G. HAMASAKA, Y. M. A. YAMADA, J. L. KATZ and Y. UOZUMI**, “Poly(*meta*-phenylene oxides) for the Design of a Tunable, Efficient, and Reusable Catalytic Platform,” *Chem. Commun.* **54**, 2878–2881 (2018).
- D. PI, H. ZHOU, Y. ZHOU, Q. LIU, R. HE, G. SHEN and Y. UOZUMI**, “Cu-Catalyzed Reduction of Azaarenes and Nitroaromatics with Diboronic Acid as Reductant,” *Tetrahedron* **74**, 2121–2129 (2018).
- G. HAMASAKA, S. ICHII and Y. UOZUMI**, “A Palladium NNC-Pincer Complex as an Extremely Efficient Catalyst Precursor for the Mizoroki–Heck Reaction,” *Adv. Synth. Catal.* **360**, 1833–1840 (2018).
- S. PAN, Y. SHUO, T. OSAKO and Y. UOZUMI**, “Controlled Aerobic Oxidation of Primary Benzylic Alcohols to Aldehydes Catalyzed by Polymer-Supported Triazine-Based Dendrimer–Copper Composites,” *Synlett* **29**, 1152–1156 (2018).
- G. SHEN, T. OSAKO, M. NAGAOSA and Y. UOZUMI**, “Aqueous Asymmetric 1,4-Addition of Arylboronic Acids to Enones Catalyzed by an Amphiphilic Resin-Supported Chiral Diene Rhodium Complex Under Batch and Continuous-Flow Conditions,” *J. Org. Chem.* **83**, 7380–7387 (2018).
- S. K. LEE, M. KONDO, G. NAKAMURA, M. OKAMURA and S. MASAOKA**, “Low-Overpotential CO_2 Reduction by Phosphine-Substituted Ru(II) Polypyridyl Complex,” *Chem. Commun.* **54**, 6915–6918 (2018).
- T. ENOMOTO, M. KONDO, M. ASADA, T. NAKAMURA and S. MASAOKA**, “Near-IR Light-Induced Electron Transfer via Dynamic Quenching,” *J. Phys. Chem. C* **122**, 11282–11287 (2018).
- T. WAKAKI, K. SAKAI, T. ENOMOTO, M. KONDO, S. MASAOKA, K. OISAKI and M. KANAI**, “C(sp³)-H Cyanation Promoted by Visible-Light Photoredox/Phosphate Hybrid Catalysis,” *Chem. –Eur. J.* **24**, 8051–8055 (2018).
- P. CHINAPANG, M. OKAMURA, T. ITOH, M. KONDO and S. MASAOKA**, “Development of a Framework Catalyst for Photocatalytic Hydrogen Evolution,” *Chem. Commun.* **54**, 1174–1177 (2018).
- T. KURAHASHI**, “Drastic Redox Shift and Electronic Structural Changes of a Manganese(III)-Salen Oxidation Catalyst upon Reaction with Hydroxide and Cyanide Ion,” *Inorg. Chem.* **57**, 1066–1078 (2018).
- H. KOJIMA, M. NAKAGAWA, R. ABE, F. FUJIWARA, Y. YAKIYAMA, H. SAKURAI and M. NAKAMURA**, “Thermoelectric and Thermal Transport Properties in Sumanene Crystals,” *Chem. Lett.* **47**, 524–527 (2018).
- Q. TAN, P. KAEWMATI, S. HIGASHIBAYASHI, M. KAWANO, Y. YAKIYAMA and H. SAKURAI**, “Triazasumanene: an Isoelectronic Heteroanalogue of Sumanene,” *Bull. Chem. Soc. Jpn.* **91**, 531–537 (2018).
- N. IKUMA, Y. YOSHIDA, Y. YAKIYAMA, N. NGAMSOMPRASERT and H. SAKURAI**, “Internal-Peripheral Diosmylation of Sumanene Overcoming the Dearomatization Hurdle by the Distortion of Curved π -System,” *Chem. Lett.* **47**, 736–739 (2018).
- Y. IIZUMI, Z. LIU, K. SUENAGA, S. OKADA, S. HIGASHIBAYASHI, H. SAKURAI and T. OKAZAKI**, “Molecular Arrangements of Corannulene and Sumanene in Single-Walled Carbon Nanotubes,” *ChemNanoMat* **4**, 557–561 (2018).
- N. NGAMSOMPRASERT, Y. YOSHIDA, Y. YAKIYAMA, N. IKUMA and H. SAKURAI**, “Nucleophilic Substitution at the Internal Carbon of Sumanene Framework with Inversion of Configuration,” *Chem. Lett.* **47**, 878–880 (2018).
- H. KOJIMA, R. ABE, F. FUJIWARA, M. NAKAGAWA, K. TAKAHASHI, D. KUZUHARA, H. YAMADA, Y. YAKIYAMA, H. SAKURAI, T. YAMAMOTO, M. IKEDA and M. NAKAMURA**, “Universality of Giant Seebeck Effect in Organic Small Molecules,” *Mater. Chem. Front.* **2**, 1276–1283 (2018).
- T. UCHIHASHI, Y. H. WATANABE, Y. NAKAZAKI, Y. YAMASAKI, T. WATANABE, T. MARUO, S. UCHIYAMA, S. SONG, K. MURATA, R. IINO and T. ANDO**, “Dynamic Structural States of ClpB Involved in Its Disaggregation Function,” *Nat. Commun.* **9**, 2147 (12 pages) (2018).

- A. NAKAMURA, T. TASAKI, Y. OKUNI, C. SONG, K. MURATA, T. KOZAI, M. HARA, H. SUGIMOTO, K. SUZUKI, T. WATANABE, T. UCHIHASHI, H. NOJI and R. IINO, "Rate Constants, Processivity, and Productive Binding Ratio of Chitinase A Revealed by Single-Molecule Analysis," *Phys. Chem. Chem. Phys.* **20**, 3010–3018 (2018).
- K. OOHORA, N. FUJIMAKI, R. KAJIHARA, H. WATANABE, T. UCHIHASHI and T. HAYASHI, "Supramolecular Hemoprotein Assembly with a Periodic Structure Showing Heme–Heme Exciton Coupling," *J. Am. Chem. Soc.* **140**, 10145–10148 (2018).
- T. MORI, S. SUGIYAMA, M. BYNE, C. H. JOHNSON, T. UCHIHASHI and T. ANDO, "Revealing Circadian Mechanisms of Integration and Resilience by Visualizing Clock Proteins Working in Real Time," *Nat. Commun.* **9**, 3245 (13 pages) (2018).
- T. UCHIHASHI, H. WATANABE and N. KODERA, "Optimum Substrates for Imaging Biological Molecules with High-Speed Atomic Force Microscopy," *Methods in Molecular Biology* **1814**, 15–179 (2108).
- M. HOSOYAMADA, N. YANAI, K. OKUMURA, T. UCHIHASHI and N. KIMIZUKA, "Translating MOF Chemistry into Supramolecular Chemistry: Soluble Coordination Nanofibers Showing Efficient Photon Upconversion," *Chem. Commun.* **54**, 6828–6831 (2018).
- M. SHIBATA, K. INOUE, K. IKEDA, M. KONNO, M. SINGH, C. KATAOKA, R. ABE-YOSHIZUMI, H. KANDORI and T. UCHIHASHI, "Oligomeric States of Microbial Rhodopsins Determined by High-Speed Atomic Force Microscopy and Circular Dichroic Spectroscopy," *Sci. Rep.* **8**, 8262 (11 pages) (2018).
- T. MARUNO, H. WATANABE, T. UCHIHASHI, S. ADACHI, K. ARAI, T. SAWAGUCHI and S. UCHIYAMA, "Sweeping of Adsorbed Therapeutic Proteins on Prefillable Syringe Enhances Subvisible Particles Generation," *J. Pharm. Sci.* **107**, 1521–1529 (2018).
- T. UMAKOSHI, H. UDAKA, T. UCHIHASHI, T. ANDO, M. SUZUKI and T. FUKUDA, "Quantum-Dot Antibody Conjugation Visualized at the Single-Molecule Scale with High-Speed Atomic Force Microscopy," *Colloids Surf., B* **167**, 264–274 (2018).
- N. TERAHARA, Y. INOUE, N. KODERA, Y. V. MORIMOTO, T. UCHIHASHI, K. IMADA, T. ANDO, K. NAMBA and T. MINAMINO, "Insight into Structural Remodeling of the FlhA Ring Responsible for Bacterial Flagellar Type III Protein Export," *Sci. Adv.* **4**, eaao7054 (9 pages) (2018).
- A. ODA, S. NAGAO, M. YAMANAKA, H. WATANABE, T. UCHIHASHI, I. UEDA, N. SHIBATA, Y. HIGUCHI and S. HIROTA, "Construction of a Triangle-Shaped Trimer and a Tetrahedral Structure Using an α -Helix-Inserted Circular Permutant of Cytochrome c555," *Chem. –Asian J.* **13**, 964–967 (2018).
- S. HISAMITSU, N. YANAI, H. KOUNO, E. MAGOME, M. MATSUKI, T. YAMADA, A. MONGUZZI and N. KIMIZUKA, "Two-Dimensional Structural Ordering in a Chromophoric Ionic Liquid for Triplet Energy Migration-Based Photon Upconversion," *Phys. Chem. Chem. Phys.* **20**, 3233–3240 (2018).
- M. MATSUKI, T. YAMADA, S. DEKURA, H. KITAGAWA and N. KIMIZUKA, "Enhancement of Ionic Conductivity in Organic Ionic Plastic Crystals by Introducing Racemic Ammonium Ions," *Chem. Lett.* **47**, 497–499 (2018).
- H. NAGATOMI, N. YANAI, T. YAMADA, K. SHIRAIISHI and N. KIMIZUKA, "Synthesis and Electric Properties of a Two-Dimensional Metal–Organic Framework Based on Phthalocyanine," *Chem. –Asian J.* **24**, 1806–1810 (2018).
- T. SHIMONO, M. MATSUKI, T. YAMADA, M. MORIKAWA, N. YASUDA, T. FUJIGAYA and N. KIMIZUKA, "Selective Ionic Conduction in Choline Iodide/Triiodide Solid Electrolyte and Its Application to Thermocell," *Chem. Lett.* **47**, 261–264 (2018).
- M. MATSUKI, T. YAMADA, N. YASUDA, S. DEKURA, H. KITAGAWA and N. KIMIZUKA, "Non-Polar to Polar Phase Transition of a Chiral Ionic Plastic Crystal and the Switch of Rotation Symmetry," *J. Am. Chem. Soc.* **140**, 291–297 (2018).
- H. ZHOU, T. YAMADA and N. KIMIZUKA, "Thermo-Electrochemical Cells Empowered by Selective Inclusion of Redox-active Ions by Polysaccharides," *Sustainable Energy Fuels* **2**, 472–478 (2018).
- R. MIYAKE, C. KUWATA, M. UENO and T. YAMADA, "Humidity Responsive ON/OFF Switching of Gas Inclusion Using Cooperative Opening/Closing of Heterogeneous Crystalline Cavities in a Peptide Ni(II)-Macrocyclic," *Chem. –Eur. J.* **24**, 793–797 (2018).

Research Center of Integrative Molecular Systems

- A. MUKAIYAMA, Y. FURUIKE, J. ABE, E. YAMASHITA, T. KONDO and S. AKIYAMA, "Conformational Rearrangements of the C1 Ring in KaiC Measure the Timing of Assembly with KaiB," *Sci. Rep.* **8**, 8803 (10 pages) (2018).
- S. AKIYAMA, A. MUKAIYAMA, J. ABE and Y. FURUIKE, "Cyanobacterial Circadian Clock System: How and Why Can It Be So Slow and Stable?" *Biological Clocks: with reference to suprachiasmatic nucleus*, 73–77 (2017).
- Y.-R. LIN, N. KOGA, S. M. VOROBIEV and D. BAKER, "Cyclic Oligomer Design with De Novo $\alpha\beta$ -Proteins," *Protein Sci.* **26**, 2187–2194 (2017).
- Y. KAWAKAMI, T. AMANO, Y. YONEYAMA, Y. AKAMINE, H. ITOH, G. KAWAGUCHI, H. M. YAMAMOTO, H. KISHIDA, K. ITOH, T. SASAKI, S. ISHIHARA, Y. TANAKA, K. YONEMITSU and S. IWAI, "Non-Linear Charge Oscillation Driven by Single-Cycle Light-Field in an Organic Superconductor," *Nat. Photonics* **12**, 474–478 (2018).
- E. TISSEROND, J. N. FUCHS, M. O. GOERBIG, P. AUBAN-SENZIER, C. MEZIERE, P. BATAIL, Y. KAWASUGI, M. SUDA, H. M. YAMAMOTO, R. KATO, N. TAJIMA and M. MONTEVERDE, "Aperiodic Quantum Oscillations of Particle-Hole Asymmetric Dirac Cones," *EPL* **119**, 67001 (5 pages) (2017).
- F. YANG, M. SUDA and H. M. YAMAMOTO, "Fabrication and Operation of Monolayer Mott FET at Room Temperature," *Bull. Chem. Soc. Jpn.* **90**, 1259–1266 (2017). (Selected of BCSJ Award Article)
- H. YAMAKAWA, T. MIYAMOTO, T. MORIMOTO, T. TERASHIGE, H. YADA, N. KIDA, M. SUDA, H. M. YAMAMOTO, R. KATO, K. MIYAGAWA, K. KANODA and H. OKAMOTO, "Mott Transition by an Impulsive Dielectric Breakdown," *Nat. Mater.* **16**, 1100–1105 (2017).

Center for Mesoscopic Sciences

- M. HOSHINA, N. YOKOSHI, H. OKAMOTO and H. ISHIHARA**, “Super-Resolution Trapping: A Nanoparticle Manipulation Using Nonlinear Optical Response,” *ACS Photonics* **5**, 318–323 (2018).
- S. HASHIYADA, T. NARUSHIMA and H. OKAMOTO**, “Imaging Chirality of Optical Fields near Achiral Metal Nanostructures Excited with Linearly Polarized Light,” *ACS Photonics* **5**, 1486–1492 (2018).
- K. MASUDA, R. SHINOZAKI, Y. KINEZUKA, J. LEE, S. OHNO, S. HASHIYADA, H. OKAMOTO, D. SAKAI, K. HARADA, K. MIYAMOTO and T. OMATSU**, “Nanoscale Chiral Surface Relief of Azo-Polymers with Nearfield OAM Light,” *Opt. Express* **26**, 22197–22207 (2018).
- K. Q. LE and H. OKAMOTO**, “Circular Polarization Dissymmetry of Two Photon-Induced Photoluminescence from Chiral Plasmonic Nanostructured Metasurfaces,” *Proc. SPIE* **10712**, 1071214 (3 pages) (2018).
- S. HASHIYADA, T. NARUSHIMA and H. OKAMOTO**, “Active Polarization Control of Optical Fields Localized on Gold Nano-Rectangles,” *Proc. SPIE* **10712**, 107121S (2 pages) (2018).
- L. ZHENG, A. KAUSAS and T. TAIRA**, “Drastic Thermal Effects Reduction Through Distributed Face Cooling in a High Power Giant-Pulse Tiny Laser,” *Opt. Mater. Express* **7**, 3214–3221 (2017).
- Y. SATO, J. AKIYAMA and T. TAIRA**, “Process Design of Microdomains with Quantum Mechanics for Giant Pulse Lasers,” *Sci. Rep.* **7**, 10732 (11 pages) (2017).
- K. NAWATA, S. HAYASHI, H. ISHIZUKI, K. MURATE, K. IMAYAMA, Y. TAKIDA, V. YAHIA, T. TAIRA, K. KAWASE and H. MINAMIDE**, “Effective Terahertz Wave Parametric Generation Depending on the Pump Pulse Width Using a LiNbO₃ Crystal,” *IEEE Trans. Terahertz Sci. Tech.* **7**, 617–620 (2017).
- R. MORIMOTO, T. GOTO, T. TAIRA, J. PRITCHARD, M. MINA, H. TAKAGI, Y. NAKAMURA, P. B. LIM, H. UCHIDA and M. INOUE**, “Randomly Polarised Beam Produced by Magnetooptically Q-Switched Laser,” *Sci. Rep.* **7**, 15398 (6 pages) (2017).
- V. YAHIA and T. TAIRA**, “High Brightness Energetic Pulses Delivered by Compact Microchip-MOPA System,” *Opt. Express* **26**, 8609–8618 (2018).
- S. JOLY, M.-A. LEMESRE, B. LEVRIER, C. LYSZYK, B. PLANO, A. COURJAUD, T. TAIRA and L. BECHOUAE**, “A Quantitative Thermal and Thermomechanical Analysis for Design Optimization and Robustness Assessment of Microassembled High Power Yb:CaF₂ Thin-Disk Laser,” *Opt. Laser Tech.* **105**, 229–241 (2018).
- H. ISHIZUKI, V. YAHIA and T. TAIRA**, “Characteristics of Crystal Quartz for High-Intensity, Sub-Nanosecond Wavelength Conversion,” *Opt. Mater. Express* **8**, 1259–1264 (2018).
- H. SHIRAI, F. KUMAKI, Y. NOMURA and T. FUJI**, “High-Harmonic Generation in Solids Driven by Sub-Cycle Mid-Infrared Pulses from Two-Color Filamentation,” *Opt. Lett.* **43**, 2094–2097 (2018).